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Karl Christe (ERC) et al., "Nitrogen Fluoride Chemistry" (abstract)

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ACS Meeting

(Statement A)

(20 August 2002, Boston, MA)

## Nitrogen Fluoride Chemistry

Ashwani Vij<sup>1</sup>, William Wilson<sup>1</sup>, Vandana Vij<sup>1</sup>, F. Tham<sup>2</sup>, M. Gerken<sup>3</sup>, and **Karl Christe<sup>4</sup>**. (1) Air Force Research Laboratory, Edwards AFB, CA 93524, ashwani.vij@edwards.af.mil, (2) University of California, Riverside, (3) University of Southern California, Los Angeles, (4) Air Force Research Laboratory, Edwards and University of Southern California, Los Angeles, Edwards AFB, CA 93524, Fax: 661-275 5471, karl.christe@edwards.af.mil

The isomerization of trans- $N_2F_2$  to cis- $N_2F_2$  going through  $N_2F^+AsF_6^-$  is unpredictable, erratic, requires 2 steps, and consumes an equimolar amount of  $AsF_5$ . It was found that catalytic amounts of  $SbF_5$  at 30C can achieve this isomerization, but still result in substantial  $N_2F_2$  losses due to  $N_2F^+SbF_6^-$  formation. When the reaction is carried out at 60C, surprisingly  $NF_4^+SbF_6^-$  .nSbF $_5$  is formed. The crystal structures of  $N_2F^+SbF_6^-$  (disordered),  $N_2F^+SbF_6^-$  (disordered),  $N_2F^+Sb_2F_{11}^-$  (ordered), and  $NF_4^+Sb_2F_{11}^-$  were determined and are discussed.  $AlF_3$  was also studied as a catalyst for the  $N_2F_2$  isomerization and was found to be an ideal catalyst resulting in very high conversions of trans- $N_2F_2$  and high yields of cis- $N_2F_2$ . The  $AlF_3$  can be used repeatedly without loss of activity or  $N_2F^+$  salt formation. Cis- $N_2F_2$  forms with  $SnF_4$  at low temperatures a 2:1 salt,  $(N_2F^+)2SnF_6^{-2}$ , that slowly loses  $N_2F_2$  at room temperature to give  $N_2F^+SnF_5$ . The crystal structure of  $H_3NF^+CF_3SO_3^-$  was also determined and exhibits a relatively long N-F bond.

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